The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1867-55

College of Soil Physics

22 October - 9 November, 2007

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Introduction

There is a great class of physical, chemical and biological phenomena that, when observed and numerically quantified, result in a sequence of data distributed along time and/or space. Time data sequences are called time series. Examples are: a) monthly average values of air temperature at a given location, b) yearly average values of rainfall for a given location, c) yearly sugarcane yield data for a given field and d) yearly soil organic matter contents for a given site. Similarly, space data sequences are called space series. Examples are: a) soil temperature values collected across a landscape at the same time, b) soil water content values collected across a corn field on the same day, c) sugarcane yield values measured across a field during a single harvest and d) soil pH values collected across a pasture in a given year.

Because these kinds of series were first analyzed in terms of a time series, we introduce the subject through sequences of data collected along time t at a given location. For a space series of data x observed at a given time, the concepts introduced here are also valid if x is substituted by t.

A discrete time or temporal series can be considered as a set of observations Y described by

$$Y(t_i) \qquad i = 1,2,3,....., n \qquad (1)$$

evaluated at equidistant times t

$$t_i - t_{i-1} = \alpha \qquad (2)$$

and manifest a serial dependence among themselves. Series collected continuously during a given time intervals ($n\alpha$) have to be transformed into a discrete series through a "sampling" procedure at equidistant time intervals. The interval α between observations is, in general, chosen by the scientist, however, in several situations it is defined by the available data set. For a given time interval, the smaller α the greater the number of observations n, allowing for a more detailed analysis of the phenomenon. According to Tukey (1980), the basic objectives for analyzing a time series are: a) modeling of the process under consideration, b) obtaining conclusions in statistical terms and c) evaluation of the model ability in terms of forecast.

When planning an investigation involving statistical methodologies, special care must be taken with sampling procedures and data preparation. Depending on the objectives of the investigation, several potential problems regarding the measurements should be avoided, or at least minimized. Among them are the stationarity of the set, data transformations, lost or “irregular” observations, outliers and short amplitudes.

The models used to describe temporal series are stochastic processes controlled by probabilistic laws. The choice of these models depends on several factors such as the behavior of the phenomenon or the “a priori” knowledge we have about its nature, and the objective of the analysis. From a practical point of view, the choice also depends on the existence of good estimation methods and on the availability of adequate software.

A temporal (spatial) series can be analyzed in two ways: 1) in the time (space) domain and 2) in the frequency domain. In both cases we wish to construct models for the series based on known concepts. For the time (space) domain models, the analysis should identify the stationary components (aleatory or purely random variables) and the nonstationary components which define the mean function of the process. In the time (space) domain the models are parametric with a finite number of parameters. Among the parametric models we find are, for example, autoregressive models AR, moving average models MA, autoregressive moving average models ARMA, autoregressive integrated moving average models ARIMA and state-space models. For the frequency domain, the models are non-parametric, and the procedures involve the decomposition of the series into frequency components with the existence of a spectrum being a fundamental characteristic. Among these models in which periodic phenomena of the data are analyzed, spectral and cospectral analyses have several applications in the soil-plant-atmosphere system.

When interested in the analysis of a series in the time (or space) domain, one of the most frequent assumptions is that the series is stationary, which means that the series develops in an aleatory or purely random way along time (or space) with their statistical properties (mean and variance) being constant reflecting some sort of a stable equilibrium. Most of the series we come across in practice, however, manifest some sort of non-stationarity. Hence, whenever a statistical procedure relies on the assumption of stationarity, it is usually necessary to transform the original data in order to satisfy the stationarity assumption.

With the simple definition of time series given above, “Time Series Analysis” becomes a well-defined area within statistics, since data that are independent and identically distributed are clearly discarded, but that are commonly used in classical statistics models. Hence, classical statistics and the statistical analysis of data that present serial dependence complement each other, one not excluding the other, and questions answered by one cannot necessarily be answered by the other.

Until recently, research in agronomy relied on classical statistics (analysis of variance, mean, coefficient of variation, regression analysis, etc), which presupposes the independence of observations among themselves and ignores the sampling locations in the field. Commonly, agronomic experiments are carried out ignoring the fact that observations might be spatially or temporally dependent. More recently it has been emphasized that adjacent observations of a given variable are not necessarily independent, and that the variability has to be taken into consideration in their statistical analysis. Nielsen and Alemi (1989) comment that observations within and among treatments might not, in fact, be independent among themselves, rendering the experimental design inadequate.

Soil spatial variability occurs at different scales and is related to variations of the parent material, climate, relief, organisms and time, i.e., related to the processes of soil formation and/or effects of management practices adopted for each agricultural use (McGraw, 1994). Statistical tools like autocorrelograms, crosscorrelograms, semivariograms, spectral analysis, kriging, co-kriging, autoregressive models, ARIMA models, state-space models, etc, are now frequently used to study the spatial variability of soil attributes, and can potentially lead to management practices that allow a better understanding of the interactive processes within the soil-plant-atmosphere system (Vieira et al., 1981; Vieira et al., 1983; Wendroth et al., 1997; Dourado-Neto et al., 1999; Vieira, 2000; Webster and Oliver, 2001; Wendroth et al., 2001; Nielsen and Wendroth, 2003; Timm et al., 2003; Reichardt and Timm, 2004; Timm et al., 2006).

The concern about the spatial variability of soil properties is expressed in several reports related to agronomy. Until recently, the most detailed studies of this variability indicated limitations of the classical methods of Fisher´s statistics. In general, normality and independence of observations are not tested, even knowing that the independence must be assumed a priori, i.e., before sampling. All variability is assumed to be residual, being due to uncontrolled factors. Recently, applied statistical tools now take into consideration the structure of the spatial dependence of the observations. This approach has lead to an improvement in the understanding of physical, chemical and biological processes that control the soil-plant-atmosphere system and, therefore, to the adoption of better management practices with less environmental impact. Having this in mind, we now present the basic principles of concepts and tools most commonly used to analyze and characterize the spatial variability of agronomic data sets.

Autocorrelation Function ACF

After sampling a variable Y, its mean and variance are calculated to reflect the sampled population, assuming that the set is representative and obtained randomly. In many cases the observations are not independent of each other, and it is possible to calculate an autocorrelation coefficient, which plotted as a function of the distance between observations will indicate their level of auto-dependence. For stationary processes (those in which the static properties are independent of space or time), the covariance between observations is a function of the number of lags h between their sampling points. Time series are collected along time at intervals of α (equation 2) minutes, hours, months, etc, and space series along transects (or grids) at spacings of α ($x_i - x_{i-1} = \alpha$), in cm, m, km, etc. The covariance between such variables given by Salas et al. (1988) is

$$C(h) = \frac{1}{n-h}\sum_{i=1}^{n-h}\left[Y(x_{i+h}) - \overline{Y}\right]\left[Y(x_i) - \overline{Y}\right] \qquad (3)$$

If C(h) is normalized dividing it by the variance s^2 of the sample, we obtain the coefficient r(h) of the autocorrelation function

$$r(h) = \frac{C(h)}{s^2} \qquad (4)$$

which manifests values between +1 and -1. It is important to note that for the calculation of r(h), the observations Y have to be collected at regularly spaced intervals. The values of r(h) for h = 0, which represents the correlation between $Y(x_i)$ and $Y(x_i)$ is obviously equal

to 1. For the first neighbor pairs $Y(x_i)$ and $Y(x_{i+1})$ for a distance of one lag α (h = 1), a value of r(1) can be obtained using equations (3) and (4). The same procedure is used for second neighbor pairs [$Y(x_i)$ and $Y(x_{i+2})$], and further neighbors (h = 3, 4, ...) obtaining a r(h) value for each h. Plotting r as a function of h we obtain the autocorrelogram of the variable Y.

The next step is the calculation of the fiducial intervals of r, to recognize if they are significant or not, and in this way define the length interval αh in which the spatial dependence of the variable is significant. One way to measure the autocorrelation confidence interval CI is using the accumulated probability function (e.g., ± 1.96 for a 95% probability level) for the normalized distribution function (Davis, 1986), and the number of observations (n-h). Therefore,

$$CI = \pm \frac{p}{\sqrt{n - h}} \qquad (5)$$

Crosscorrelation function CCF

Having two sets of variables $Y(x_i)$ and $W(x_i)$ observed at the same locations x_i (or same times t_i), their spatial crosscorrelation structure can be analyzed calculating coefficients of crosscorrelation. Although each variable has its own autocorrelogram, an analysis of their crosscorrelation indicates to which distance (or time interval) one is related to the other. The coefficient r_c of the crosscorrelation function will be also a function of h, and describes the degree of linear association between both variables (Davis, 1986; Shumway, 1988; Wendroth et al., 1997).

The coefficients of the crosscorrelation function $r_c(h)$, between the variables Y and W, separated by distances αh, or by a lag number h, are calculated with

$$r_c(h) = \frac{cov_{YW}(h)}{s_Y \times s_W} \tag{6}$$

where

$$cov_{YW}(h) = \frac{1}{n-h} \sum_{i=1}^{n-h} \left[Y(x_i) - \overline{Y}\right]\left[W(x_{i+h}) - \overline{W}\right] \tag{7}$$

and s_Y^2 is the variance of Y

$$s_Y^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left[Y(x_i) - \overline{Y}\right]^2 \tag{8}$$

and s_W^2 is the variance of W

$$s_W^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left[W(x_i) - \overline{W}\right]^2 \tag{9}$$

A plot of r_c as a function of h represents the crosscorrelogram. For h = 0 (observations taken at the same position x_i), the value $r_c(0)$ given by equation (6) is the linear regression coefficient obtained through classical statistics. For the first neighbor pairs

[$Y(x_i)$, $W(x_{i+1})$] collected at a distance α in one direction (h = 1), we obtain the coefficient r_c (1), and for the other direction (h = -1) the coefficient r_c(-1). This is because in the case of two variables, each of them has different neighbors for each direction, i.e., we have two pairs – (Y_i, W_{i+1}) and (Y_i, W_{i-1}). The same procedure is used for more distant neighbors, obtaining values of r_c(h) and r_c(-h). A crosscorrelogram indicates how far two different observations are spatially related (Wendroth et al., 1997).

According to Nielsen & Wendroth (2003), it is more difficult to estimate the significance of r_c(h) as compared to r(h). Significance tests like the t test are usually based on the assumption that the observed values of $Y(x_i)$ and $W(x_i)$ are normally distributed and independent among themselves. Taking this into consideration, the significance level of r_c is, in general, given by

$$t = \sqrt{\frac{(n-h)-2}{1-r_c^2}} \qquad (10)$$

where (n-h) is the number of pairs used for the calculation of r_c. The level of significance of the test is obtained by comparing the value of t in equation (10) with critical values of t for (n-2) degrees of freedom. The crosscorrelation function is, in general, not symmetric, i.e., $r_c(h) \neq r_c(-h)$. Note that in the case of the autocorrelation there is symmetry, r(h) = r(-h)., when there is a physical relation between Y and W, the crosscorrelogram will tend to symmetry (Nielsen & Wendroth, 2003).

The State-Space Approach

The state-space model of a stochastic process involving j data sets $Y_j(x_i)$, all collected at the same locations is based on the property of Markovian systems that establishes the independence in the future of the process in relation to its past, once given the present state. In these systems, the state of the process condenses all information of the past needed to forecast the future.

The state-space model is a combination of two systems of equations. The first is the observation equation

$$\mathbf{Y_j}(\mathbf{x_i}) = \mathbf{M_{jj}}(\mathbf{x_i})\,\mathbf{Z_j}(\mathbf{x_i}) + \mathbf{v_{Y_j}}(\mathbf{x_i}) \tag{11}$$

where observation vector $\mathbf{Y_j(x_i)}$ of the process is generated as a function of the state vector $\mathbf{Z_j(x_i)}$. The second is the state equation

$$\mathbf{Z_j}(\mathbf{x_i}) = \phi_{jj}\,\mathbf{Z_j}(\mathbf{x_{i-1}}) + \mathbf{u_{Z_j}}(\mathbf{x_i}) \tag{12}$$

where the non observed state vector $\mathbf{Z_j(x_i)}$ is dynamically evolved.

The matrix $\mathbf{M_{jj}}$ in equation (11) comes from the following set of linear observation equations

$$\begin{aligned}
Y_1(x_i) &= m_{11}Z_1(x_i) + m_{12}Z_2(x_i) + \ldots\ldots\ldots\ldots + m_{1j}Z_j(x_i) + v_{Y_1}(x_i)\\
Y_2(x_i) &= m_{21}Z_1(x_i) + m_{22}Z_2(x_i) + \ldots\ldots\ldots\ldots + m_{2j}Z_j(x_i) + v_{Y_2}(x_i)\\
&\vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\qquad \vdots \qquad\quad \vdots \qquad\quad \vdots\\
Y_j(x_i) &= m_{j1}Z_1(x_i) + m_{j2}Z_2(x_i) + \ldots\ldots\ldots\ldots + m_{jj}Z_j(x_i) + v_{Y_j}(x_i)
\end{aligned}$$

which can be written in the matrix form

$$\begin{bmatrix} Y_1(x_i) \\ Y_2(x_i) \\ \vdots \\ Y_j(x_i) \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \ldots\ldots\ldots m_{1j} \\ m_{21} & m_{22} \ldots\ldots\ldots m_{2j} \\ \vdots & \vdots \quad\quad \vdots \\ m_{j1} & m_{j2} \ldots\ldots\ldots m_{jj} \end{bmatrix} \times \begin{bmatrix} Z_1(x_i) \\ Z_2(x_i) \\ \vdots \\ Z_j(x_i) \end{bmatrix} + \begin{bmatrix} v_{Y_1}(x_i) \\ v_{Y_2}(x_i) \\ \vdots \\ v_{Y_j}(x_i) \end{bmatrix}$$

The matrix $\boldsymbol{\phi_{jj}}$ in equation (12) comes from the following set of state equations

$$\begin{aligned} Z_1(x_i) &= \phi_{11} Z_1(x_{i-1}) + \phi_{12} Z_2(x_{i-1}) + \ldots\ldots\ldots\ldots + \phi_{1j} Z_j(x_{i-1}) + u_{Z_1}(x_i) \\ Z_2(x_i) &= \phi_{21} Z_1(x_{i-1}) + \phi_{22} Z_2(x_{i-1}) + \ldots\ldots\ldots\ldots + \phi_{2j} Z_j(x_{i-1}) + u_{Z_2}(x_i) \\ &\vdots \quad\quad \vdots \quad\quad\quad \vdots \quad\quad\quad\quad\quad \vdots \quad\quad \vdots \quad\quad \vdots \\ Z_j(x_i) &= \phi_{j1} Z_1(x_{i-1}) + \phi_{j2} Z_2(x_{i-1}) + \ldots\ldots\ldots\ldots + \phi_{jj} Z_j(x_{i-1}) + u_{Z_j}(x_i) \end{aligned}$$

or in the matrix form:

$$\begin{bmatrix} Z_1(x_i) \\ Z_2(x_i) \\ \vdots \\ Z_j(x_i) \end{bmatrix} = \begin{bmatrix} \phi_{11} & \phi_{12} \ldots\ldots\ldots \phi_{1j} \\ \phi_{21} & \phi_{22} \ldots\ldots\ldots \phi_{2j} \\ \vdots & \vdots \quad\quad \vdots \\ \phi_{j1} & \phi_{j2} \ldots\ldots\ldots \phi_{jj} \end{bmatrix} \times \begin{bmatrix} Z_1(x_{i-1}) \\ Z_2(x_{i-1}) \\ \vdots \\ Z_j(x_{i-1}) \end{bmatrix} + \begin{bmatrix} u_{Z_1}(x_i) \\ u_{Z_2}(x_i) \\ \vdots \\ u_{Z_j}(x_i) \end{bmatrix}$$

The observation vector $\mathbf{Y_j(x_i)}$ is related to the state vector $\mathbf{Z_j(x_i)}$ through the observation matrix $\mathbf{M_{jj}(x_i)}$ and by the observation error $\mathbf{v_{Yj}(x_i)}$ (equation 11). On the other hand, the state vector $\mathbf{Z_j(x_i)}$ at position i is related to the same vector at position i-1 through

the state coefficient matrix $\boldsymbol{\phi_{jj}(x_i)}$ (transition matrix) and an error associated to the state $\boldsymbol{u_{Zj}(x_i)}$ with the structure of a first order autoregressive model. It is assumed that $v_j(x_i)$ and $u_j(x_i)$ are normally distributed and independent as well as being non correlated among themselves for both lags.

The above equations contain distinct perturbations or noises, one associated with observations $v_{Yj}(x_i)$ and the other with state $u_{Zj}(x_i)$. According to Gelb (1974), the development of methods to process noise-contaminated observations can be credited to the work carried out by Gauss and Legendre (around 1800) who both independently developed the method of the minimum squares for the linear models. More recently, Plackett (1950) developed a recursive solution for the minimum square method in linear models. Kalman (1960) using a state-space formulation, developed a very good recursive filter for estimations in stochastic, dynamic linear systems, being well known today as the Kalman Filter KF. According to Gelb (1974), a good estimator is a computational algorithm that processes observations in order to find a minimum estimate (following some sort of optimization criterion) of the state error of a system, using: a) the knowledge of the dynamics of the observations and of the system, b) assuming statistical inferences for the noises associated to observations and to states and c) knowledge of the initial condition of the information. In summary, given a dynamic system of equations that describes the behavior of the vectors of state and of observations, the statistic models that characterize the observational and state errors, and an initial condition of the information, the KF performs the sequential actualization of the state vector at time (or space) i-1 to time (or space) i. It can therefore be said, that the KF is essentially a recursive solution that permits a sequential processing of the observations, within the original method of the minimum

squares of Gauss. It should be noted however, that another algorithm has to be used [for example, the algorithm of maximum likelihood (EM) thoroughly discussed in Shumway and Stoffer (2000)] so that, together with the KF, the problem of noise-contaminated observations can be solved (Gelb, 1974).

Depending on the objectives of a study involving the state-space methodology, one can have three different types of estimates: a) when the time (or space) at which an estimate is wished coincides with the last observed value, the problem is said to be one of filtering; b) when the time (or space) of interest is inside the set of observations, i.e., the complete set of data is used to estimate the point of interest, the problem is said to be one of smoothing; and c) when the time (or space) of interest is after the last observation, the problem is said to be one of forecasting.

From this it can be seen that any linear or non-linear model (Katul et al., 1993; Wendroth et al., 1993) can be represented in the state-space formulation, i.e., by a system of two equations: one for the observations vector and another for the evolution of the state vector.

The state-space approach can also be used like the kriging and co-kriging (Alemi et al., 1988; Deutsch and Journel, 1992) to interpolate data spatially (or temporally). However, the philosophy behind these tools is different. For kriging and co-kriging the condition of stationarity of the data is required, which is not the case in state-space (Shumway, 1985).

The linear system of dynamic equations (11 and 12) has been presented here in a generalized form of the state-space approach. Now we shall present two different ways of using this approach, the first presented by Shumway (1988) which has been used by several researchers in agronomy, giving emphasis to the equation of the evolution of the state of the

system (equation 12); and the second, introduced by West and Harrison (1989, 1997) which is still not so frequently used in agronomy, giving greater emphasis to the observation equation (11). Applications of these two different state-space approaches can be found in Morkoc et al. (1985), Hui et al. (1998), Timm et al. (2003a), Wendroth et al. (2003) and Timm et al. (2006).

Shumway's State-Space Approach

This approach, presented by Shumway (1988) and Shumway and Stoffer (2000), gives more attention to the equation of the evolution of the state of the system, where the matrix of the transition coefficients ϕ in equation (12) is a matrix of dimension jxj that indicates the spatial measure of the linear association among the variables of interest. These coefficients are optimized through a recursive procedure, using an algorithm of the KF type (Shumway and Stoffer, 1982) in which the method of maximum likelihood is used together with the mean maximization algorithm of Dempster et al. (1977). In this case, equations (11 and 12) are solved assuming initial values for the mean and the variance of each variable in the covariance matrix **R** of the noise of the observations, for the covariance matrix **Q** of the noise associated with the state vector, for the matrix ϕ of the transition coefficients, and for the observation matrix **M**. Because Shumway (1988) considers the matrix **M** as being an unit matrix (identity), equation (11) becomes

$$\mathbf{Y_j}(\mathbf{x_i}) = \mathbf{Z_j}(\mathbf{x_i}) + \mathbf{v}_{\mathbf{Y_j}}(\mathbf{x_i}) \qquad (11a)$$

During the development of the software ASTSA (Applied Statistical Time Series Analysis) which is used for the analysis of time (space) series, the unit matrix **M** is fixed during all steps of variable estimation. This shows the greater emphasis of this approach in being referenced to the equation of state evolution, and not to the observation equation. More specific details can be found in Shumway (1988) and Shumway & Stoffer (2000).

West and Harrison (1989, 1997) State-Space Approach

The bayesian formulation presented by West and Harrison (1989, 1997) and originally published by Harrison and Stevens (1976) has not frequently been used in agronomy. In this case a general parametric formulation is used by which the observations are linearly related to parameters (equation 11), that have a dynamic evolution according to a random walk (equation 12), with the possibility of the incorporation of uncertainties associated to the model itself and to the parameters of the model. The probabilities of the model and its parameters are continuously updated in time/space using the Bayes theorem (Cantarelis, 1980). The acceptance and use of this approach was not as quick as expected, particularly by those without a deep knowledge in statistics, due to the difficulties in establishing values (or their law of variation) for the parameters "$v_j(x_i)$" and "$u_j(x_i)$". To make this approach more accessible, Ameen and Harrison (1984) used discount factors to calculate the covariance matrix of the noise parameters $u_j(x_i)$. Discount factors relate to the relevance of the observations during the evolution of time/space – with the most recent information usually being more relevant in the modeling process. The smaller the discount factor, the less importance is given to previous information. Hence, the use of these factors assures that the stochastic influence on the evolution of the parameters (equation 12) is not directly made explicit through the noise $u_j(x_i)$. The stochastic influence is derived by the

combination of a relation that establishes only the deterministic evolution of $Z_j(x_i)$ and the random process guaranteed by the discount matrix.

In this state-space approach, the state equation describes the evolution of the regression coefficients β through a vector random walk

$$\beta_i = \beta_{i-1} + w_i \tag{15}$$

where $w_i \sim N(0,W)$ are non-correlated (white noise) (Timm et., 2006). The regression coefficients vector β is related to the observable response variable Y through the observation equation

$$Y_i = F_i \beta_i + v_i \tag{16}$$

where F_i is a known matrix containing the regressors, which reduces to a vector for unidimensional responses, and v_i are non-correlated errors with zero mean, constant variance and normal distribution.

The dynamic regression model (equations 15 and 16) is a local and not a global model, because it contains variable β coefficients having the subscript i. These coefficients vary along space according to a Markovian evolution (first order autoregressive process, not having to be stationary), being therefore called “state variables of the system” (West and Harrison, 1989, 1997; Pole et al., 1994). Hence, we have a basic regression equation (observation equation, equation 16), and a second equation (evolution equation, equation 15) which characterizes the form of the variation of these state parameters along space. Parameters are estimated in an optimal way through algorithms of the type KF (extensions of the basic KF). The equations of estimation are sequential, comprising the observational equations of actualization (via Bayes theorem and observation equation) and the spatial actualization equations (consequence of the evolution equation).

In this approach more emphasis is given to equation (11). In the dynamic regression, the β coefficients are considered as a state vector (equation 12) following a random walk process. The transition matrix ϕ is unity and the observation matrix **M** that relates the state vector with the observation vectors, being formed of the regression coefficients.

Because dynamic regression models represented in the state-space form are relatively recent tools, they have not yet been frequently used to quantify soil-plant relations. Having been introduced in the sixties, their greater implementation occurred only since the late eighties (West and Harrison, 1989, 1997). Being models of local adjustment, it is possible to precisely estimate regression coefficients for each sampled location. This possibility tends to alleviate the problem of spatial variability encountered in precision agriculture. Today, the more commonly used static models are models of global behavior with their regression coefficients being average values not varying along space. They provide an opportunity to describe the spatial association among different variables measured across a field and can, therefore, provide a better understanding of the complex relations between plant and soil variables. Inasmuch as the response of one variable is not unique in a field, the application of statistical multiple regressions oftentimes yield low coefficients of determination. Because these kinds of analyses give only a global estimate of coefficients that do not represent point to point variations and their use can lead to interpretations that induce inadequate management procedures. We conclude that dynamic regression models of state-space form are more adequate for the study of soil-plant relationships mainly because they account for the local spatial and temporal character of agronomic processes.

Acknowledgments

To CNPq and FAPERGS for financial support.

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